COSIRES 2012
Computer Simulations of Radiation Effects in Solids

Crack mechanical failure in lithium niobate crystal under ion irradiation; novel simulation by extended finite elements.

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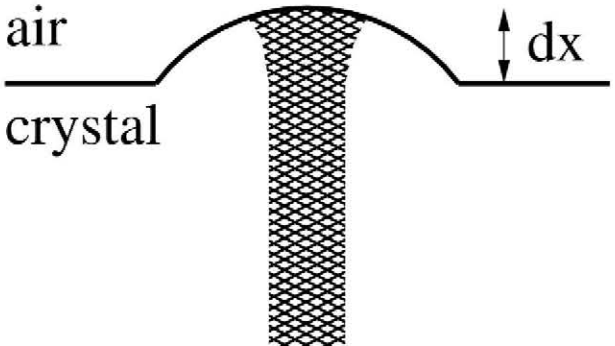
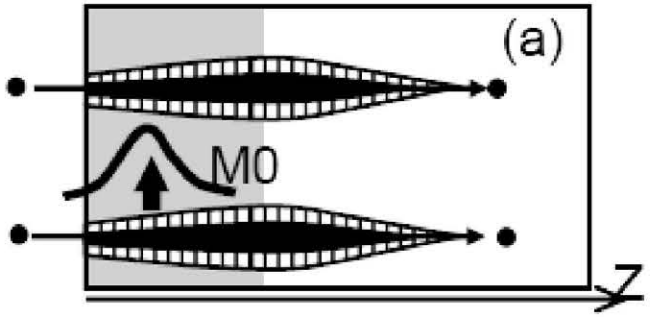
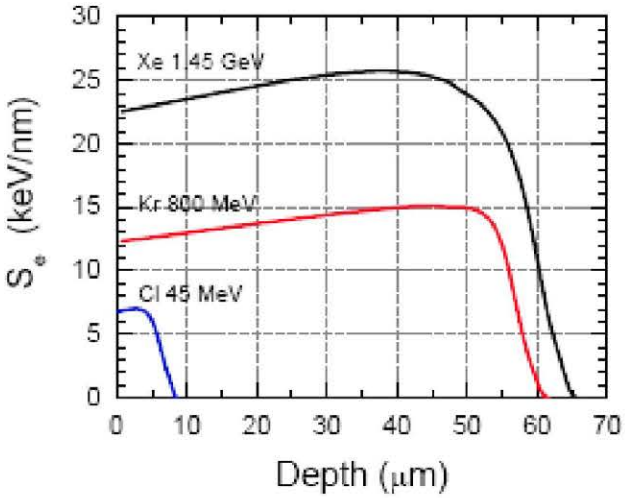
Electronic excitation effects

- Swift heavy ions produce amorphous tracks in many materials
- Mechanism dominated by electronic-excitation effects
- Marked threshold
- Hillock formation



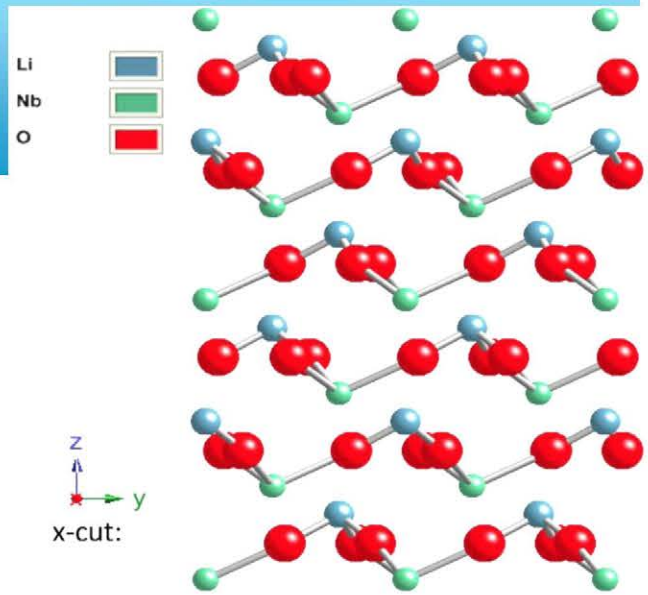


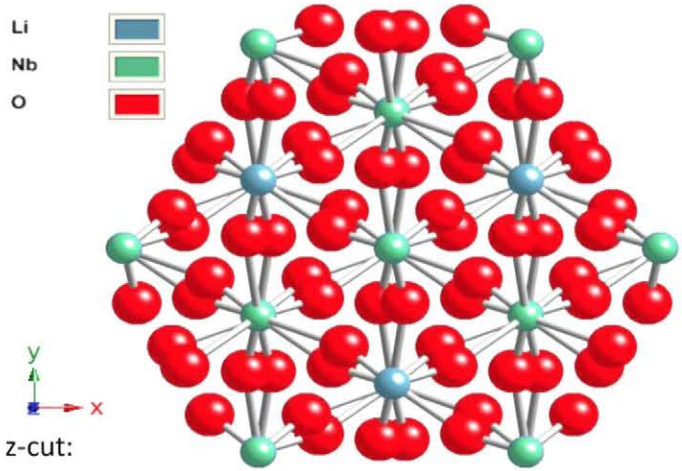


Peña-Rodríguez et al. Ch. 12 of *Ion Implantation, Ed. M. Goorsky, ISBN 978-953-51-0634-0* (2012)

Lithium Niobate

- Important optical material
- Anisotropic crystal
- Simmetry C_3
- Cut X: anisotropic
- Cut Z: almost isotropic





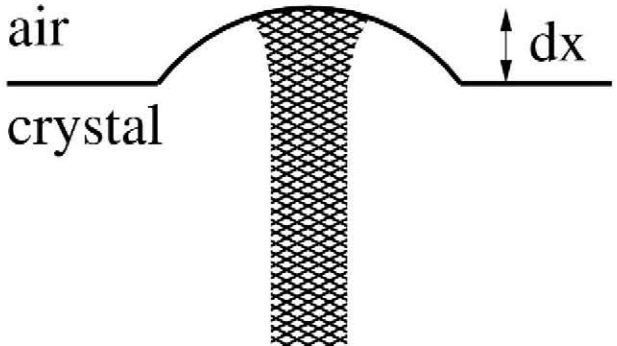
Rivera et al. J. Phys. D: Appl. Phys. 44 (2011) 475301

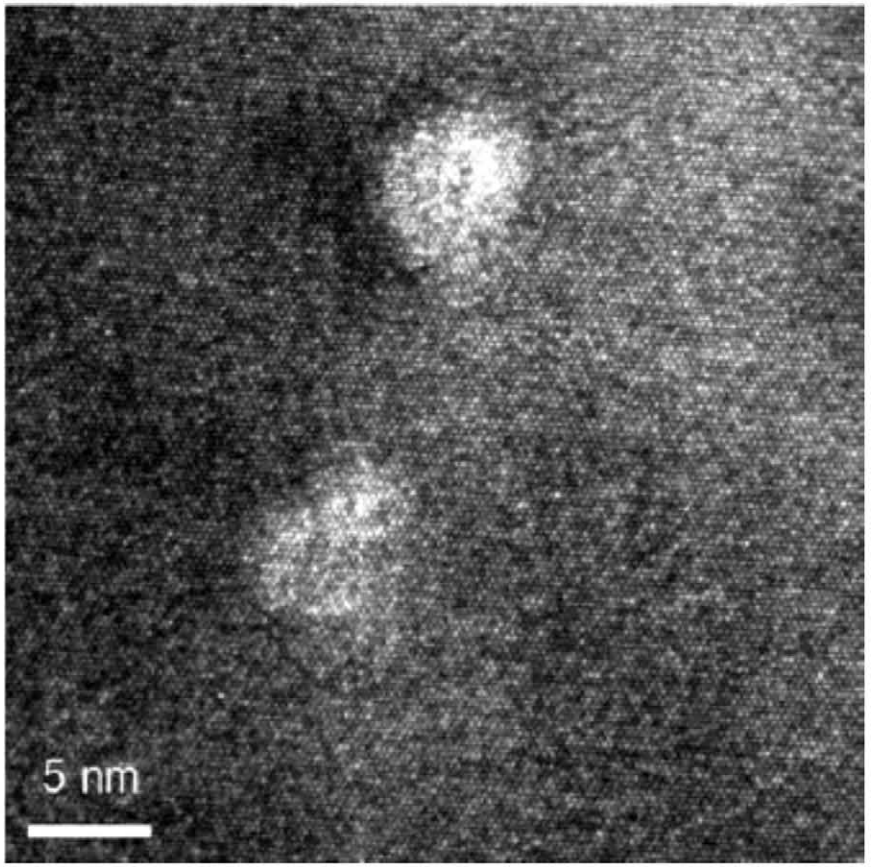
Ion-induced nano-tracks in LiNbO3

TEM: Amorphous tracks

Br 45 MeV on $LiNbO_3$
R=2.5 nm

Crespillo et al. Appl. Phys. A104, (2011) 1143

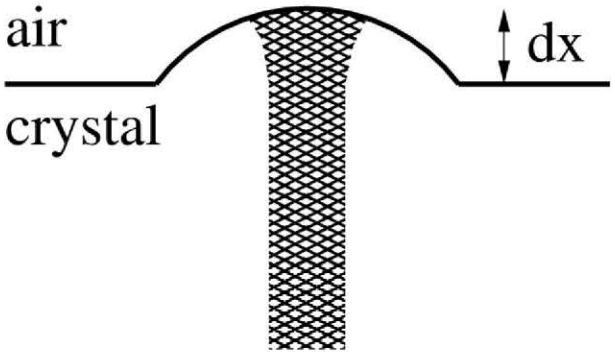


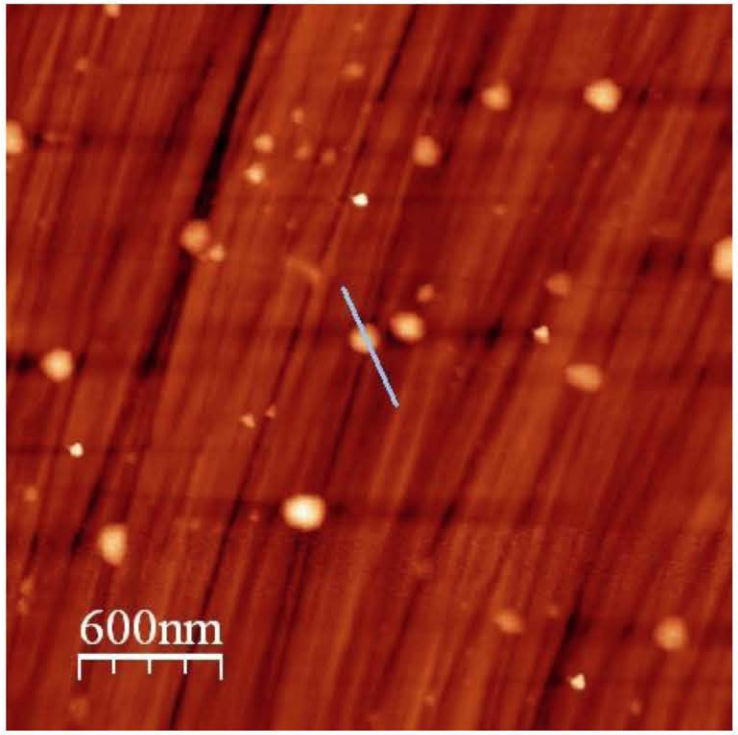


Ion-induced nano-tracks in $LiNbO_3$

AFM: Hillocks

Pb 2.3 GeV on $LiNbO_3$
dx ~ 3.5 nm





AFM: Pores (after HF etch)
Elipsoidal shape (Cut X)

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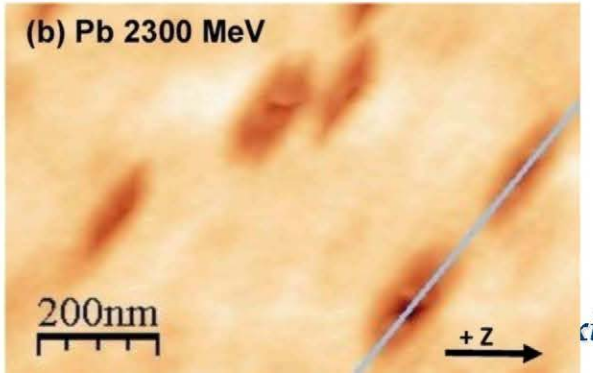

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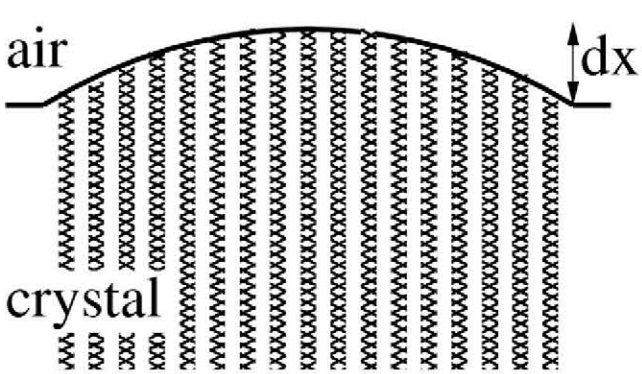
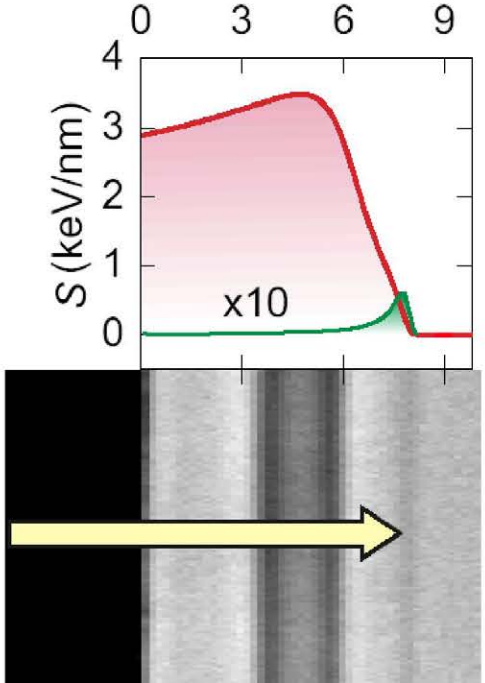
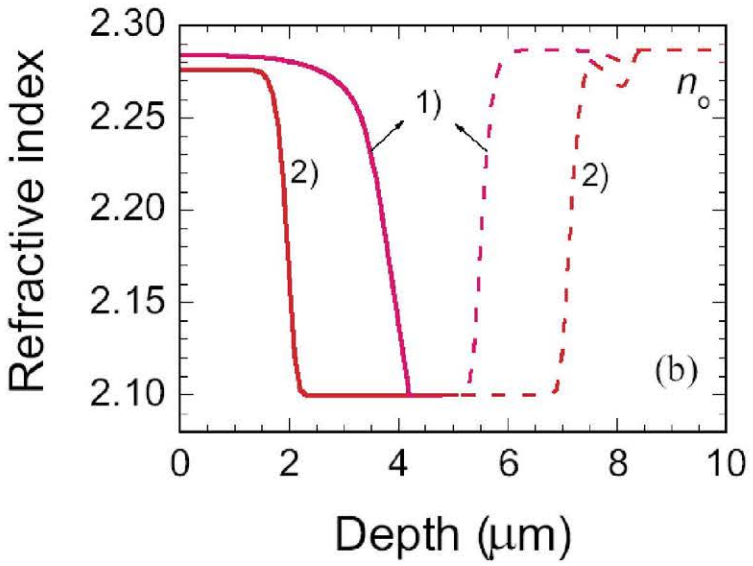
Ion-induced nano-tracks in $LiNbO_3$



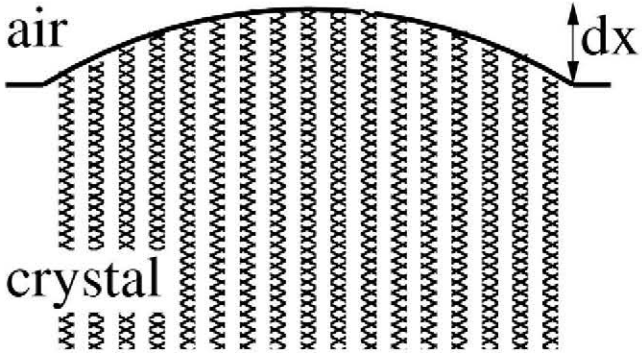
- Track overlapping leads to continuous layers and swelling
- Important effects
- Waveguides



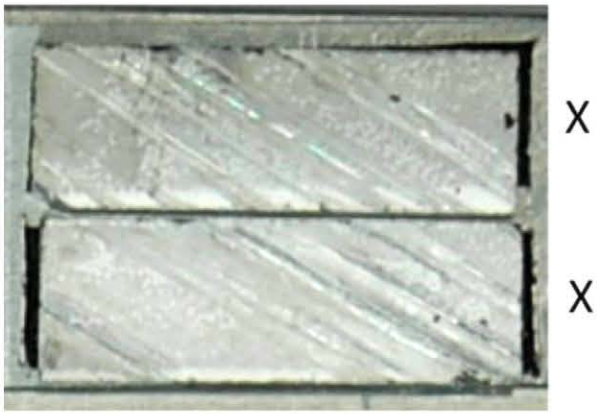


Rivera et al. PSSA 206 (2009) 1109

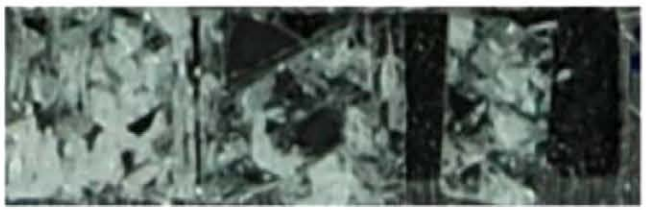
Ion-induced nano-tracks in LiNbO3



- Track overlapping leads to continuous layers and swelling
- Important effects
- Xe 11 MeV/amu : cracks
- Cut X oriented along 45°
- Cut Z not oriented



Z

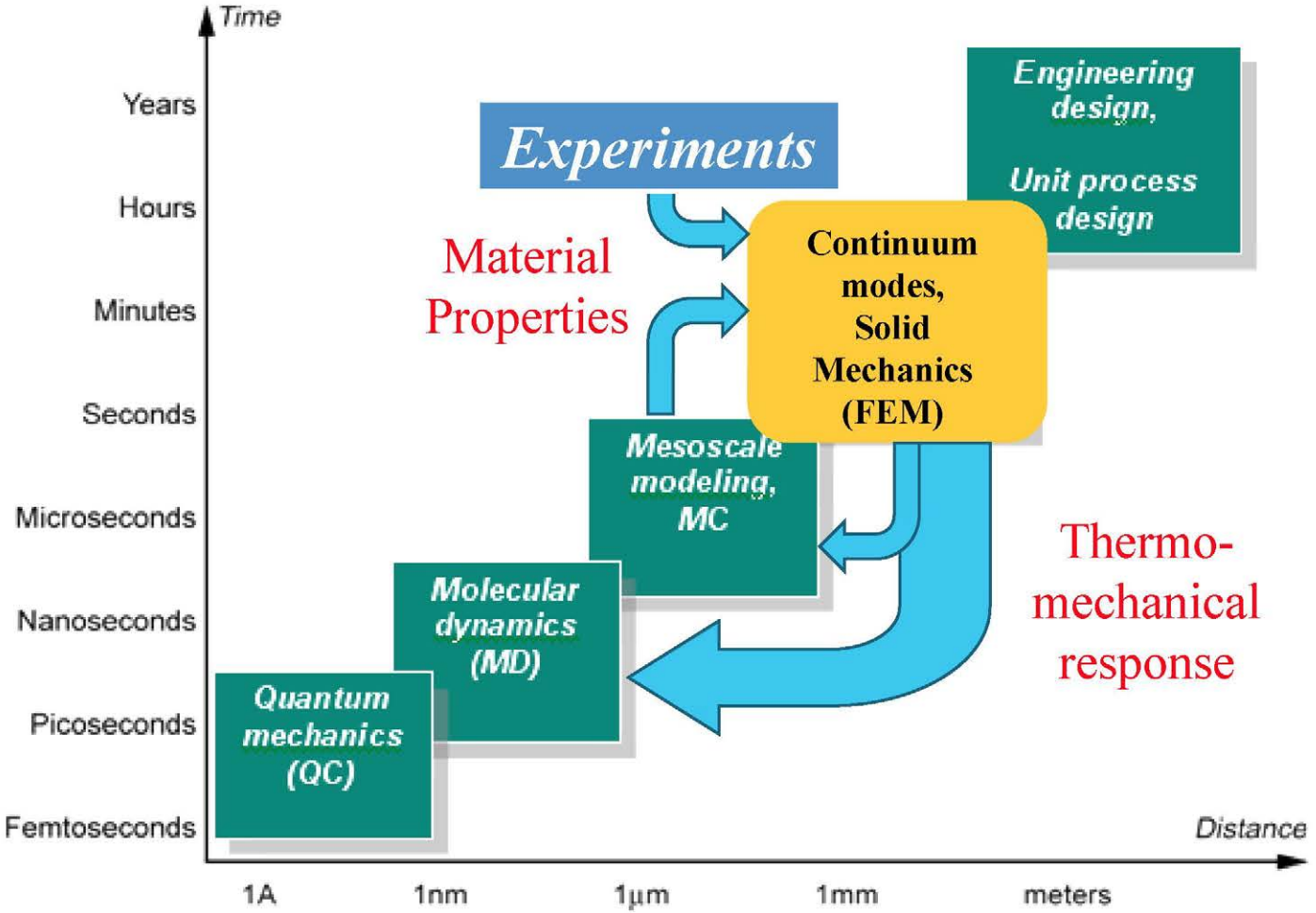


Rivera et al. J. Phys. D: Appl. Phys. 44 (2011) 475301

Ion-induced nano-tracks in $LiNbO_3$

- Amorphization beyond threshold
- Hillock and pore formation
- Anisotropy in Cut X
- Overlapping leads to continuous layers and swelling
- Cracks observed, in Cut X they are oriented

From macro to nano-scale

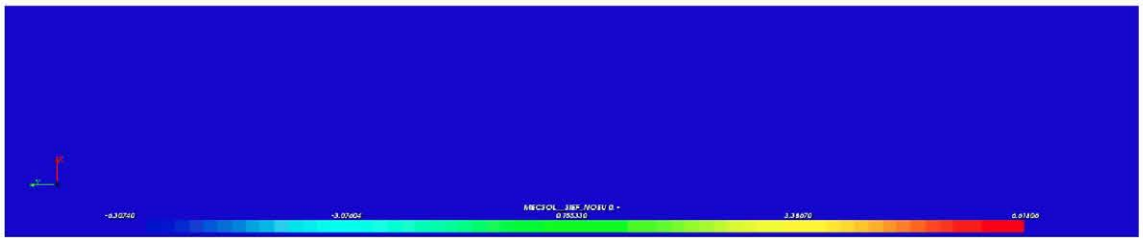


http://www.kintechlab.com/solutions/methodology/

Finite elements

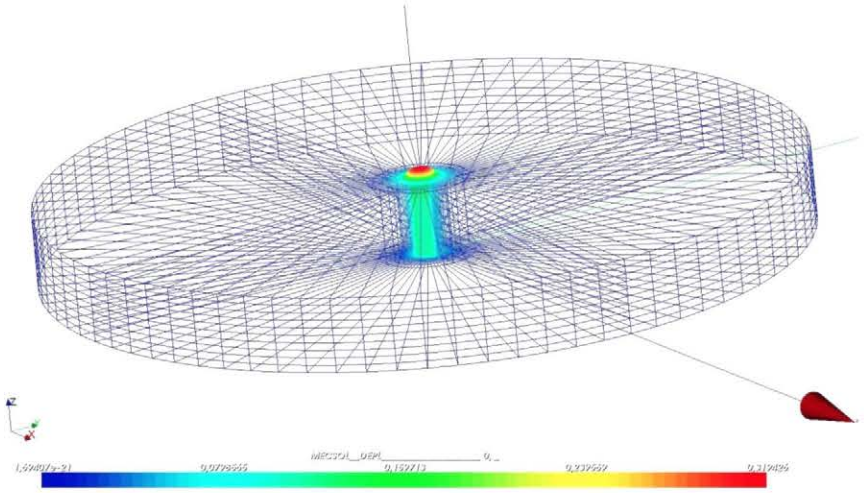
- Amorphous tracks have lower density than the crystal
- We insert a realistic cylindrical track
- Dilatation induces deformations and stresses
- A hillock per nano-track are expected at surface

6 nm radius nano-track with stress in Y direction.

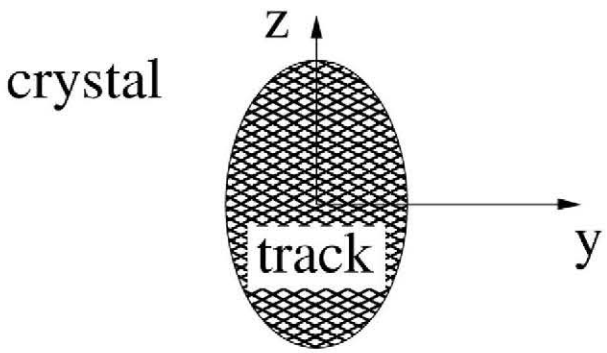


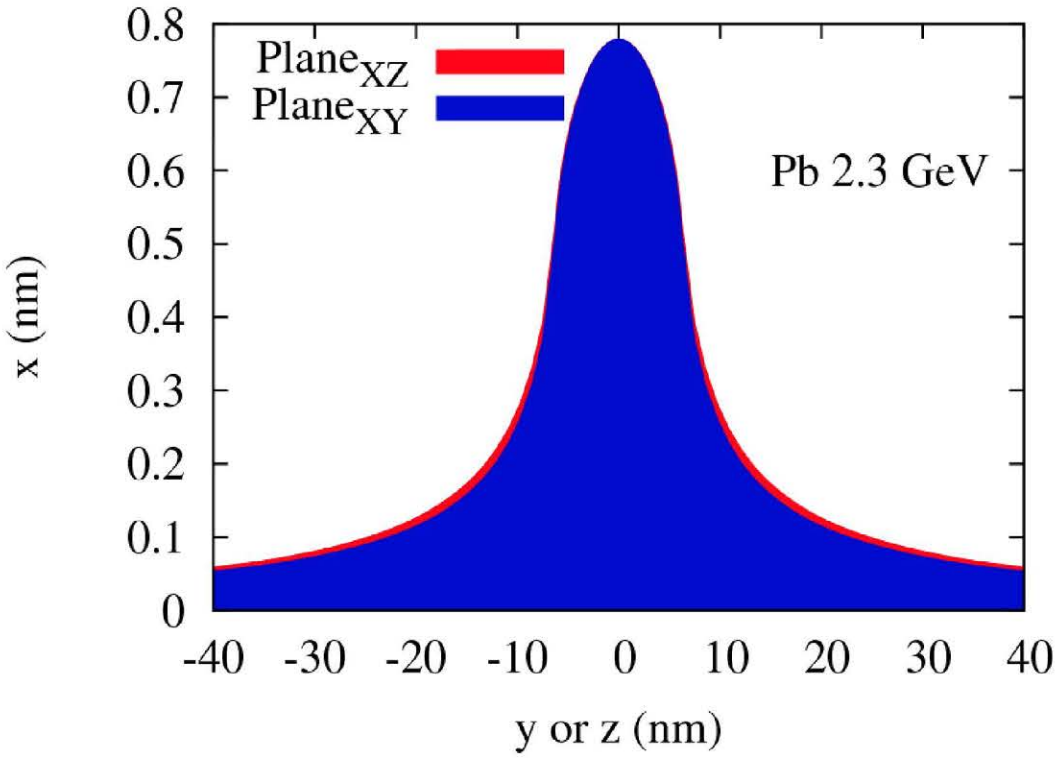
Finite element method for nano-structured materials

- Geometry simple but with a huge range of scales
- Orthotropic properties in crystal LiNbO3, and isotropic properties in amorphous track
- Boundary condition to simulate single track or multiple track (high fluence)



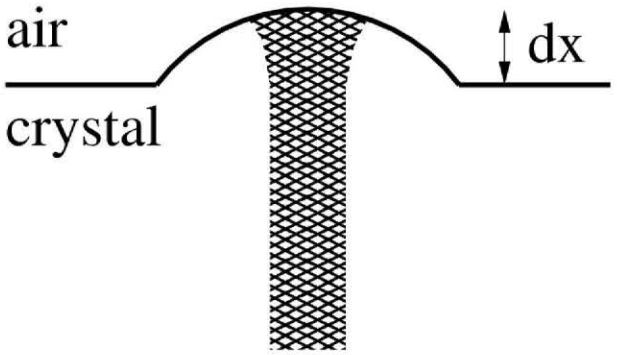
Simulations in LiNbO3

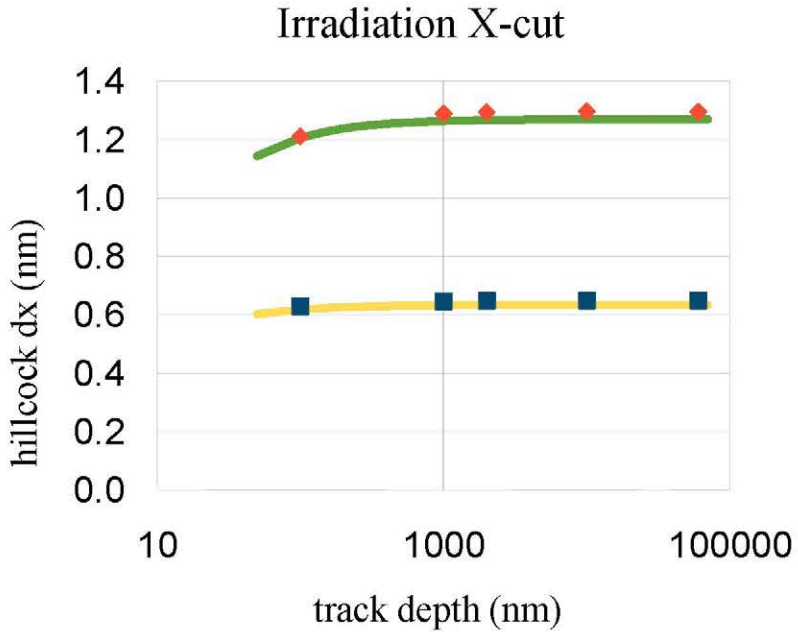




The hillock has an elliptic shape due to orthotropic properties of LiNbO3

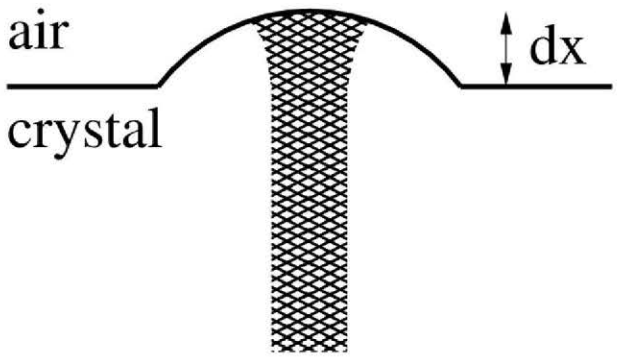
Simulations of X-cut in $LiNbO_3$

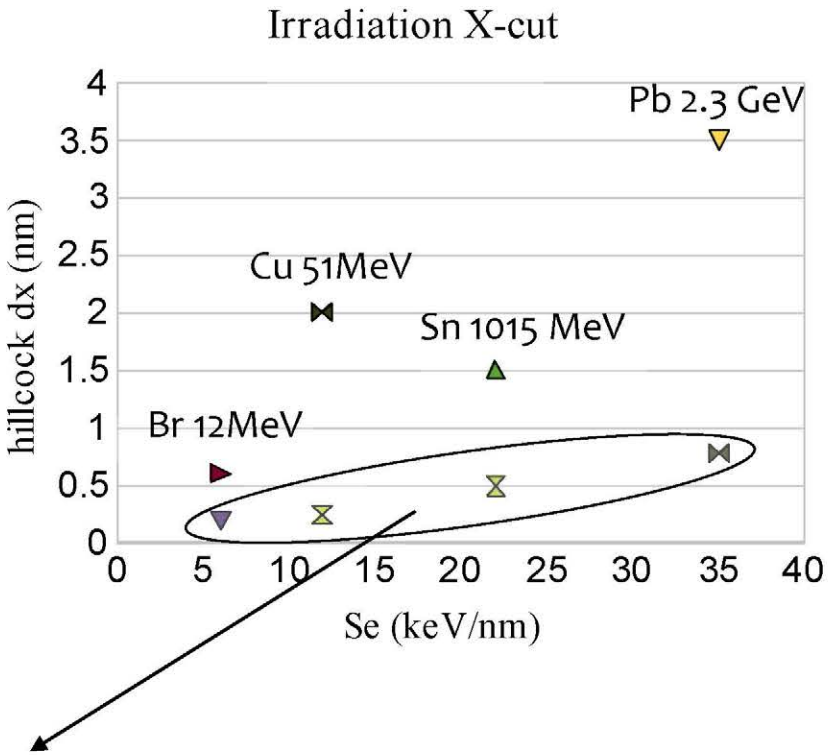




Simulations agree with analytical solution of
Colin et al. Phyl. Mag. A 81 (2001) 857...
But introducing anisotropy with strong approx.
Rivera et al. J. Phys. D: Appl. Phys. 44 (2011) 475301

Experiments versus simulations

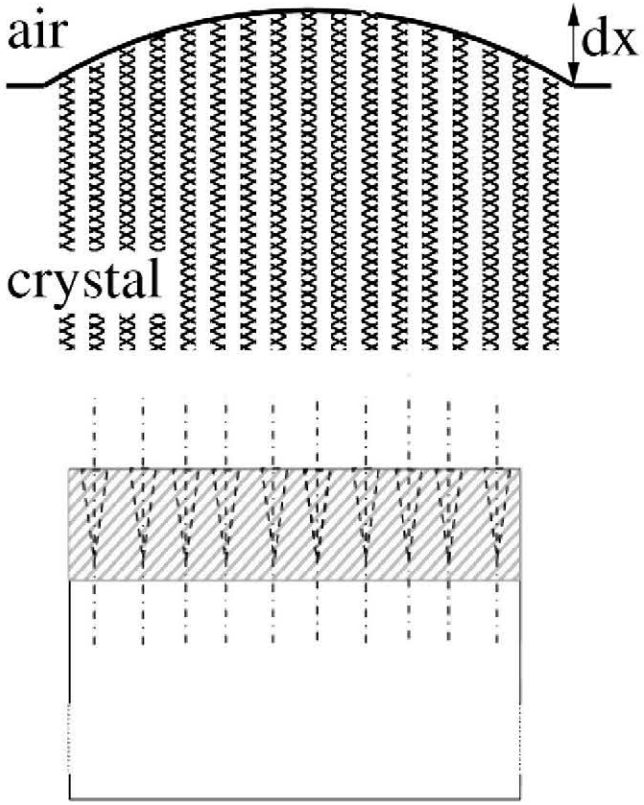


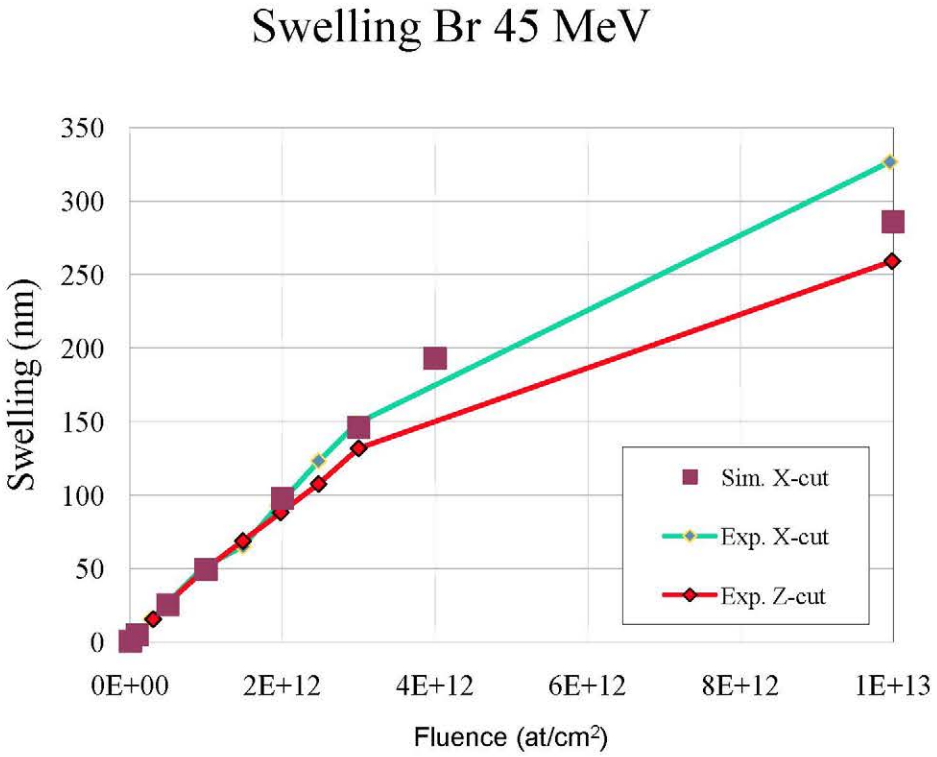


Simulation are below experimental values.

Elastic effects do not account for phase transformation

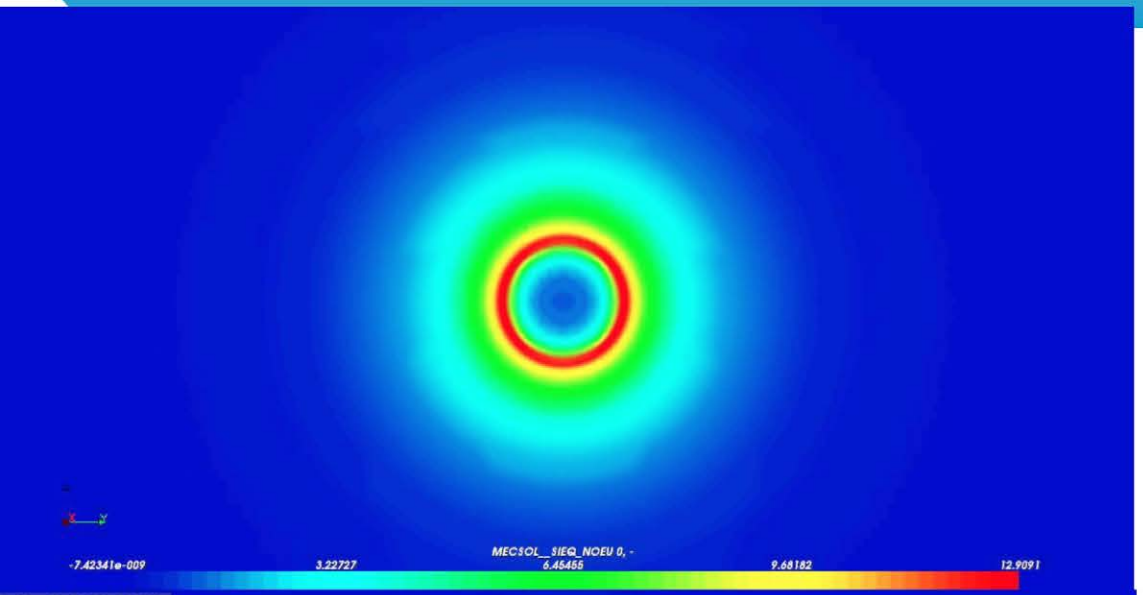
Swelling





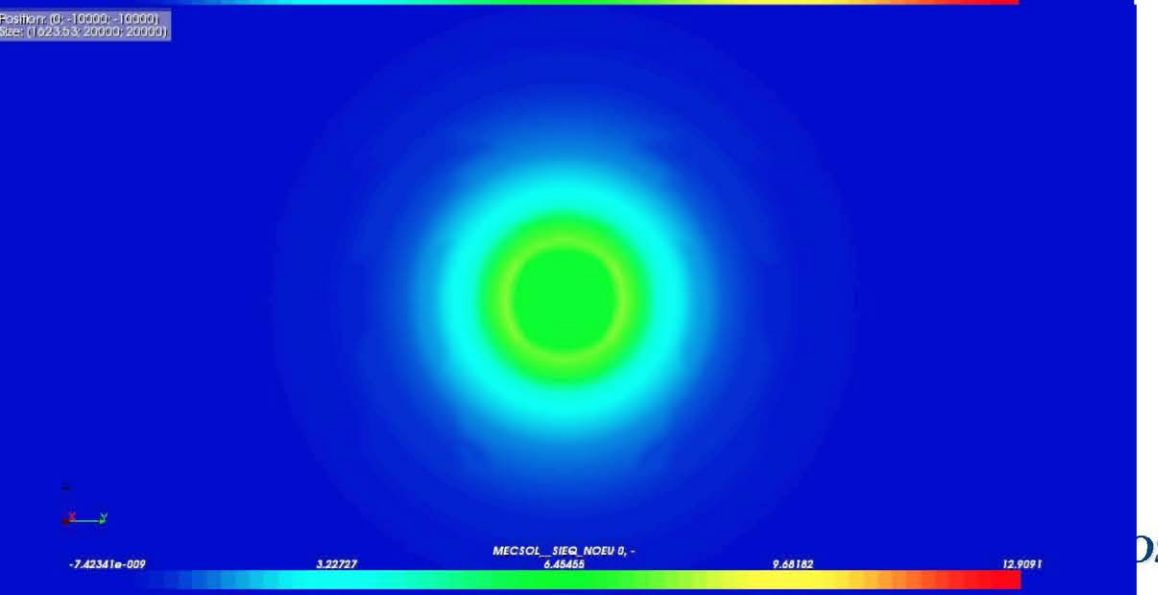
- Simple models can not simulate the process of track overlapping
- X-cut swelling simulations agree with experiments, at high fluence underestimate
- Because layer growth not considered
- Tracks considered cylindrical

Stress



Single track Br 45 MeV of 2.3 nm radius

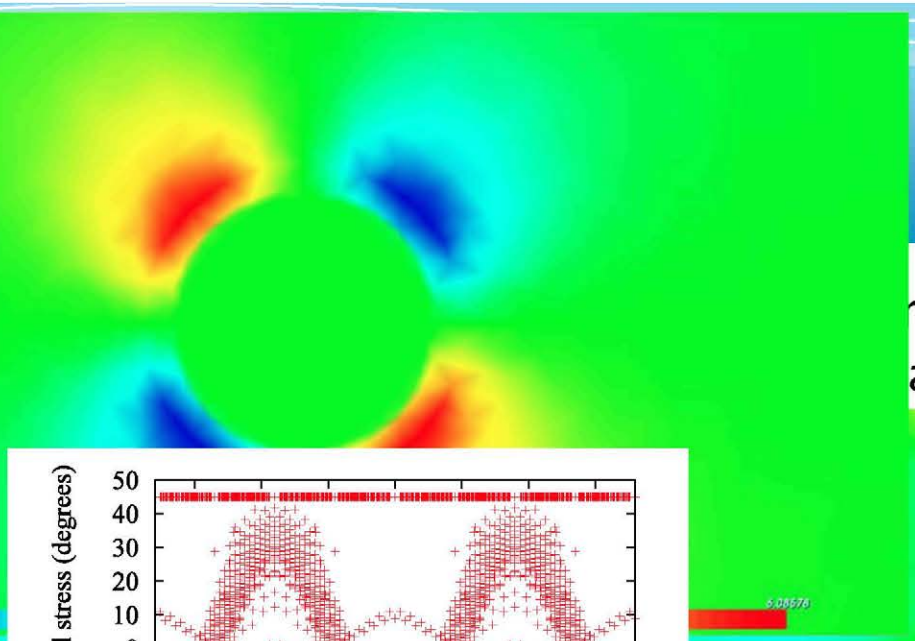
Maximum stress (12 Gpa) at the **top** surface expressed with Von Mises stress.

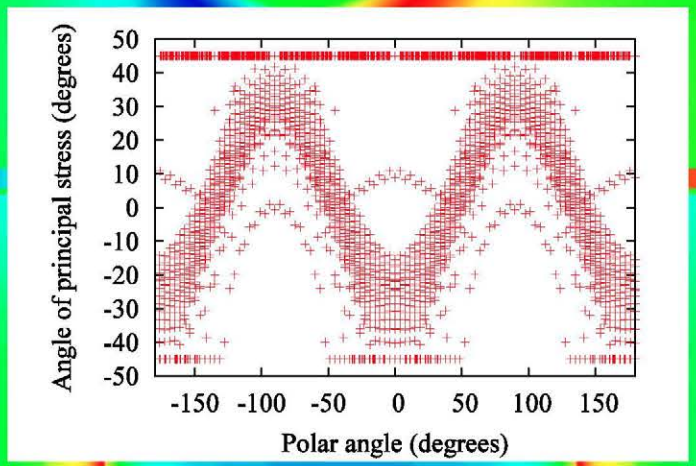


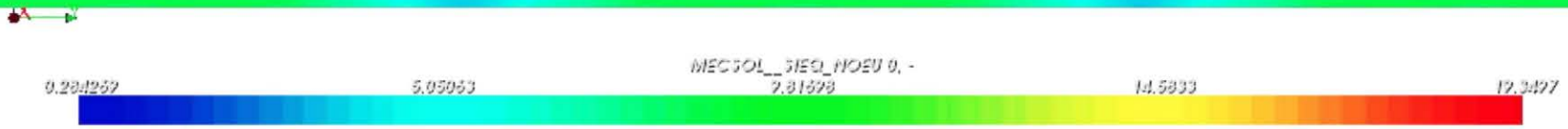
Maximum stress (9 Gpa) at the **bottom** of the sample expressed with Von Mises stress.

Instituto de Fusi

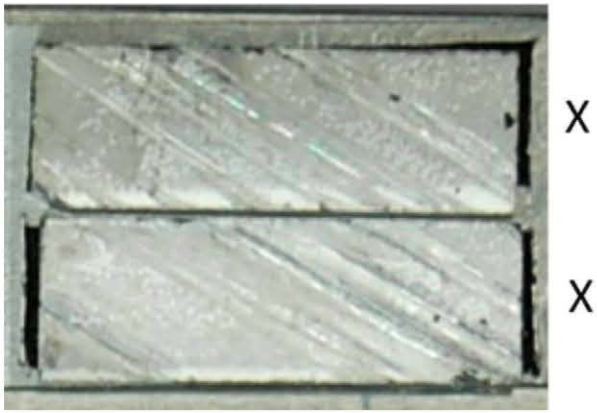
r 45 MeV of
adius







Cracks in X-cut

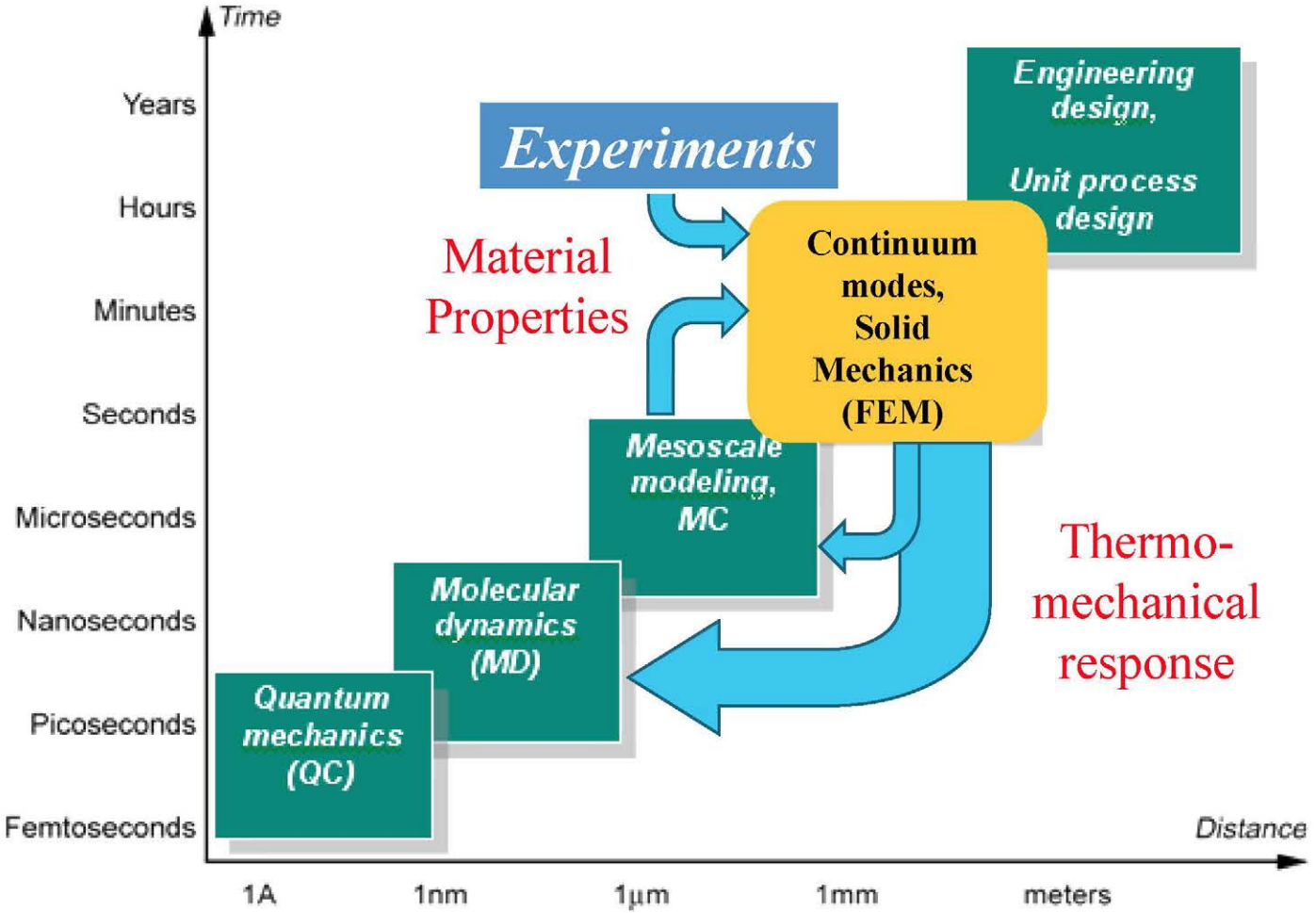


Preference direction ±45º
Corresponding to the direction of maximum stresses
FEM allow us to give yield strength

Conclusions

- ✓ Finite elements can be used in nano-scale to fill the gap between theory and experiments.
- ✓ The elastic model accounts for anisotropy in Cut X
- ✓ The elastic model can not account for the hillock height due to phase transition
- ✓ On the other hand, it explains well the results of swelling, except at high fluence probably due to extra growth of layer
- ✓ Maximum stresses at track boundary over planes forming 45°
- ✓ In progress full simulation of crack growth from seed in region of maximum stress
- ✓ In progress MD and FE studies in quartz

From macro to nano-scale



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Thanks for your attention